Error Analysis and Adaptive Localization for Ensemble Methods in Data Assimilation

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Deutscher Wetterdienst
Wetter und Klima aus einer Hand

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Challenge

- Understand the basic properties of localization in the ensemble Kalman filter scheme.
- Define an adaptive localization depending on the density of data, observation and background error.
- Decomposition of the error sources to determine its effect on the optimal localization length scale.
- Perspective of approximation theory and functional analysis.
- Addressed with numerical experimental results.

Introduction

In order to find out φ we should minimize the functional

$$J(\varphi) := \left\| \varphi - \varphi^{(b)} \right\|^2 + \left\| f - H\varphi^{(b)} \right\|^2.$$

The normal equations are obtained from first order optimality conditions

$$\nabla_{\varphi} J = 0.$$

Usually, the relation between variables at different points is incorporated by using covariances/weighted norms:

$$J(\varphi) := \| \varphi - \varphi^{(b)} \|_{B^{-1}}^2 + \| f - H\varphi \|_{R^{-1}}^2,$$

The update formula is now

$$\varphi^{(a)} = \varphi^{(b)} + BH^*(R + HBH^*)^{-1}(f - H\varphi^{(b)})$$

Ensemble Kalman Filter

- In the KF method B evolves with the model dynamics: $B_{k+1} = MB_kM^*$.
- EnKF[1] is a Monte Carlo approximation to the KF.
- EnKF methods use reduced rank estimation techniques to aproximate the classical filters.
- The ensemble matrix $Q_k := \left(\varphi_k^{(1)} - \overline{\varphi}_k^{(b)}, ..., \varphi_k^{(L)} - \overline{\varphi}_k^{(b)}\right)$.
- In the EnKF methods the background convariance matrix is represented by $B := \frac{1}{L-1} Q_k Q_k^*$.
- Update solved in a low-dimensional subspace

$$U^{(L)} := \text{span}\{\varphi_k^{(1)} - \overline{\varphi}_k^{(b)}, ..., \varphi_k^{(L)} - \overline{\varphi}_k^{(b)}\}.$$

[1] Evensen 1994

- The updates of the EnKF are a linear combination of the columns of Q_k.

$$\varphi_k - \varphi_k^{(b)} = \sum_{l=1}^{L} \gamma_l \left(\varphi_k^{(l)} - \overline{\varphi}_k^{(b)} \right) = Q_k \gamma$$

$$\varphi_k^{(a)} = \varphi_k^{(b)} + Q_k Q_k^* H^* (R + H Q_k Q_k^* H^*)^{-1} (f_k - H\varphi_k^{(b)})$$

- The previous cost function

$$J(\varphi) := \|\varphi - \varphi^{(b)}\|_{B^{-1}}^2 + \|f - H\varphi\|_{R^{-1}}^2$$

results now in this expresion to minimize:

$$J(\gamma) := \|Q_k \gamma\|_{B_k^{-1}}^2 + \|f_k - H\varphi_k^{(b)} - HQ_k\gamma\|_{R^{-1}}^2$$

- We denote the analysis error $E_k := \|\varphi^{(a)} - \varphi^{(true)}\|$

Error analysis without background contribution

Lemma

Assume that H is injective, that we study true measurement data $f = H\varphi^{(true)}$ *and consider the EnKF with data term only*

$$J^{(data)}(\gamma) = \|(f - H\varphi^{(b)}) - HQ_k\gamma\|^2_{R^{-1}}$$

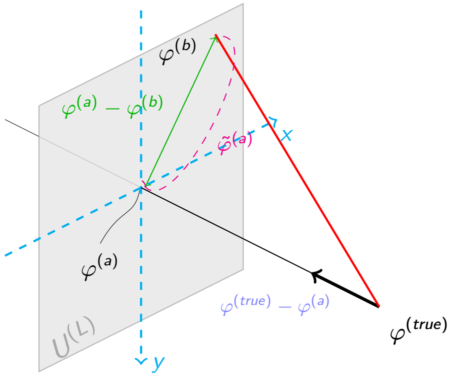
Then, for the analysis $\varphi^{(a)}$ *calculated by the EnKF the difference* $\varphi^{(a)} - \varphi^{(b)}$ *is the orthogonal projection of* $\varphi^{(true)} - \varphi^{(b)}$ *onto the ensemble space* $U_k^{(L)}$ *and the analysis error is given by* [2]

$$E_k = d_{H^* R^{-1} H}\Big(U_k^{(L)}, \varphi_k^{(true)} - \varphi^{(b)}\Big),$$

where the right-hand side denotes the distance between a point $\psi = \varphi_k^{(true)} - \varphi^{(b)}$ *and the subspace* $U^{(L)}$ *with respect to the norm induced by the scalar product* $< ., . >_{H^* R^{-1} H}$.

[2] Proof in Perianez A., Reich H. and Potthast R. *In preparation.*

Illustration of Lemma



Error analysis with background term

Theorem

For H injective, the analysis $\tilde{\varphi}^{(a)}$ generated by the minimization of the whole cost function within the EnKF for perfect data $f^{(true)}$ satisfies the estimate

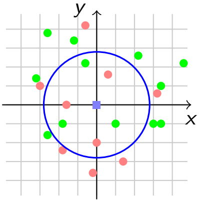
$$\begin{aligned} \left\| \tilde{\varphi}^{(a)} - \varphi^{(true)} \right\|_{HR^{-1}H} &\leq \sqrt{q^2 (E^{(b)})^2 + (1-q^2) E_{min}^2} \\ &= E^{(b)} \sqrt{q^2 + (1-q^2) \frac{E_{min}^2}{(E^{(b)})^2}} \end{aligned}$$

with some constant $q < 1$ depending on B, R and H, where

$$\begin{aligned} E_{min} &:= \min_{\varphi \in U^{(L)}} \left\| \varphi - \varphi^{(true)} \right\|_{H^* R^{-1} H} = \left\| \check{\varphi}^{(a)} - \varphi^{(true)} \right\|_{H^* R^{-1} H}, \\ E^{(b)} &:= \left\| \varphi^{(b)} - \varphi^{(true)} \right\|_{H^* R^{-1} H}. \end{aligned}$$

Localization

- Localization denotes the restriction to a subset of physical space.
- Study the analysis in dependence of the localization radius ρ when the domain D is given by a ball $D = B_\rho(x_0)$.



- Localization function χ_ρ depending on ρ such that[3]

$$\chi_\rho(x) := \begin{cases} \chi_\rho(x) & x \in D \\ 0 & \text{otherwise.} \end{cases}$$

- R localization[4] modifies the observation error covariance matrix to suppress the influences of distant observations $\rightarrow R_{loc} := \chi \cdot R$

$$E^{(\rho)}(x_0) := \left\| \breve{\varphi}^{(a,\rho)} - \varphi^{(true,\rho)} \right\|_{H^* R_{loc}^{-1} H}$$

[3] Houtekamer et al. 1998

[4] Hunt et al. 2007

Localization. Convergence results.

Theorem

We study assimilation in the case where true data $\varphi^{(true)}$ *are used and* $\hat{\varphi}^{(a,\rho)}$ *is chosen such that* $\hat{\varphi}^{(a,\rho)} - \varphi^{(b)}$ *is the orthogonal projection of* $\varphi^{(true)} - \varphi^{(b)}$ *onto the ensemble space* $U^{(L)}$*. Assume that there is* c*,* $C > 0$ *such that for all* $x \in D$ *there is* $l \in \{1, ..., L\}$ *such that*

$$|\varphi^{(l)}(x) - \varphi^{(b)}(x)| \geq c,$$

and that the ensemble members are continuously differentiable on D *with*

$$|\nabla(\varphi^{(j)}(x) - \varphi^{(b)}(x))| \leq C, \quad x \in D, \quad j \in \{1, ..., L\}.$$

Further assume that $\varphi^{(true)} - \varphi^{(b)}$ *is continuously differentiable on* D*. Then, we have*

$$\sup_{x_0 \in D} E^{\rho}(x_0) \leq \tilde{C}\rho \quad \to 0, \quad \rho \to 0$$

with some constant $\tilde{C}$ *depending on* C*,* H *and* R*.*

Remarks

- Using last two theorems we can derive

$$\left\|\tilde{\varphi}^{(a,\rho)} - \varphi^{(true,\rho)}\right\|_{H^* R_{loc}^{-1} H} \leq \sqrt{E^{(b,\rho)} q^2 + (1-q^2) C \rho^2}.$$

- The first term q^2 in the square root reflects the influence of the *background error*.
- The second *approximation error* term can be made small by reducing the localization radius ρ.
- In a balanced relationship between background and data, q is between 0 and 1.
- *Effective observation error*: With data error, ρ needs to be kept sufficiently large since it also controls the number of observations used for the assimilation.

A one-dimensional example

- Ensemble space given by linear functions
  $U^{(L)} := \{a + bx : \ \ a, b \in \mathbb{R}\} \subset L^2([0, A])$.
- The truth $\varphi^{(true)}$ given by a quadratic function
  $\varphi^{(true)}(x) := B \cdot (x - C)^2, \ \ x \in [0, A]$.
- Observations from a Gaussian distribution with variance σ_{obs}.
- Localization by a decomposition of $[0, A]$ into $q \in \mathbb{N}$ subsets
  $[A_j, A_{j+1}]$ where $A_j := \frac{j \cdot A}{q}, \ \ j = 0, ..., q$.
- Localization radius here $\rho = A/2q$.
- On each subset the analysis is carried out by solving the least squares problem in $U^{(L)}|_{[A_j, A_{j+1}]}$.

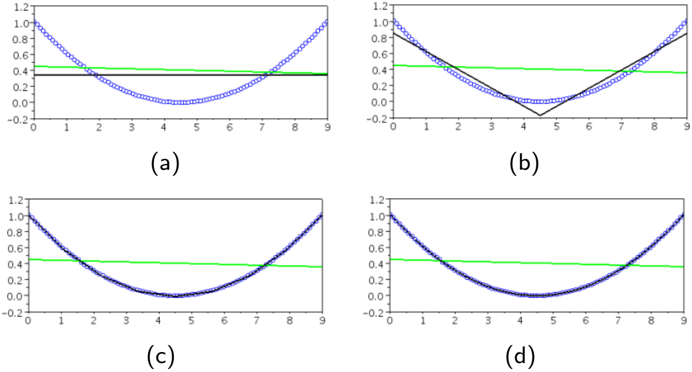


Figure: The truth (blue line) overlaps with the observations (blue circles) due to σ_{obs} takes very small values ($\sigma_{obs} = 0.0005$). The green line shows background information. In (a) we show the analysis without any localization. Localization radii gradually decreases in (b), (c), and (d).

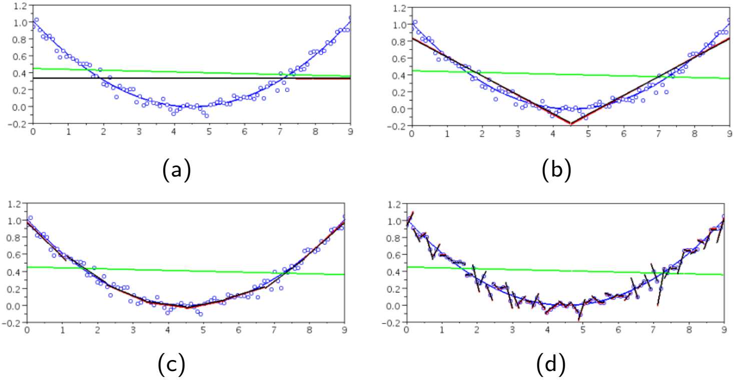


Figure: Observation error $\sigma_{obs} = 0.05$. No localization is applied for (a). In (b), (c) and (d) the localization radii is progressively reduced.

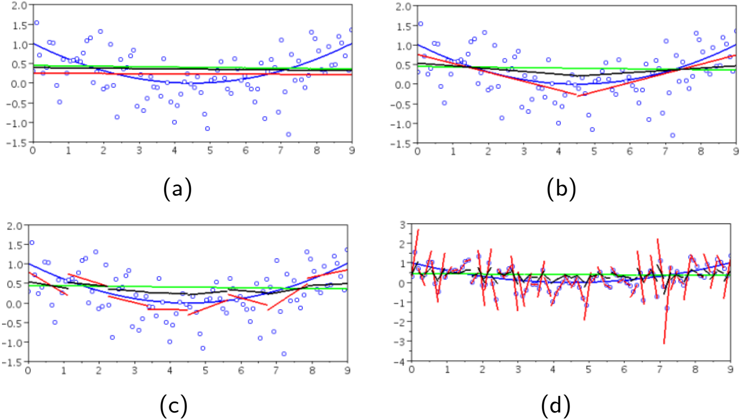


Figure: Higher observation error, $\sigma_{obs} = 0.5$, is provided. The analsyis in (a) is computed with no localization, being progressively smaller in (b), (c) and (d) cases.

Estimating fronts in a 2d example with LETKF [5]

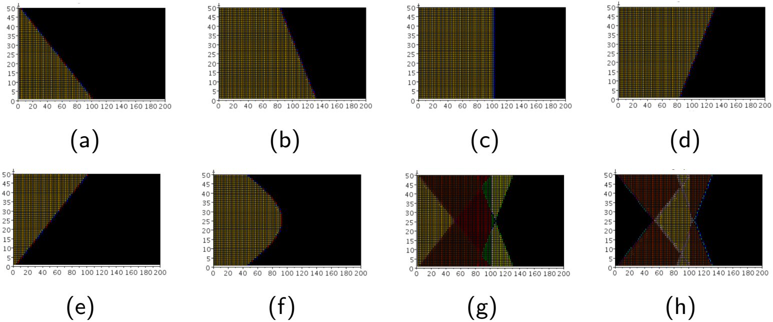


Figure: The different ensemble members are shown in (a)-(e). The truth is displayed in (f). The first guess mean and spread are plotted in (g) and (h), respectively.

[5] Hunt et al. 2007

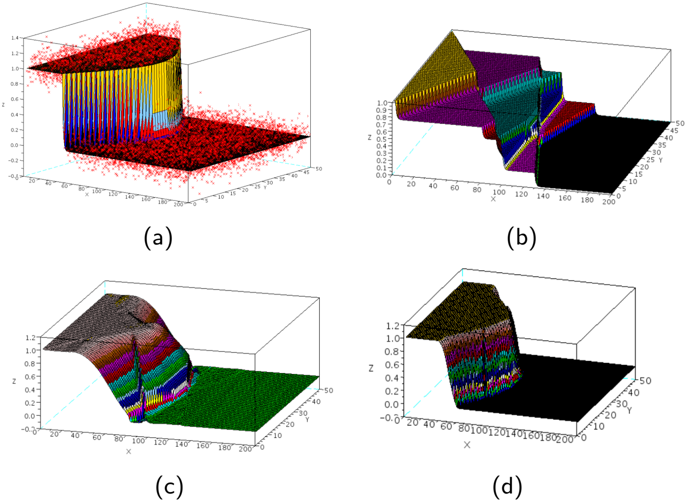
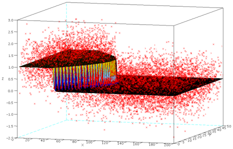
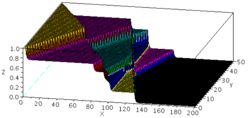


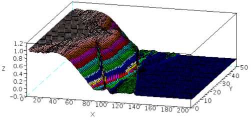
Figure: Truth (front) and observations (red crosses) for $\sigma_{obs} = 0.1$ in (a). Truth (a) is approximated without any localization procedure in (b). In (c) $\rho = 15$, and in (d) $\rho = 5$.



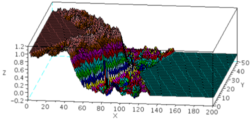
(a)



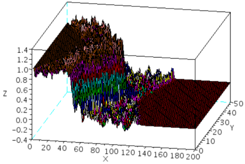
(b)



(c)



(d)



(e)

Figure: Truth and observations for $\sigma_{obs} = 0.5$. (a) is approximated without any localization in (b), with $\rho = 15$ in (c), $\rho = 5$ in (d) and $\rho = 1$ in (e).

Optimal localization radius

- Estimation of ρ_{loc} as a function of σ_{obs} and observation density μ.
- **Approximation error** (or undersampling error[6]) decreases with smaller localization radius.
- **Effective observation error** decreases with a larger ρ, as a larger number of observations gives a better statistical estimates.
- This leads to the *error asymptotics*

$$E(\rho) = \alpha\rho^p + \frac{\beta\sigma_{obs}}{\sqrt{\mu}}\rho^{-\frac{d}{2}}, \quad \rho > 0,$$

- The minimum of $E(\rho) \quad \rightarrow \quad \rho_{min} = c\left(\frac{d}{p}\right)^{\frac{2}{d+2p}}$ with $c(\alpha, \beta, p, \sigma_{obs}, \mu)$

[6] Oke et al. 2007

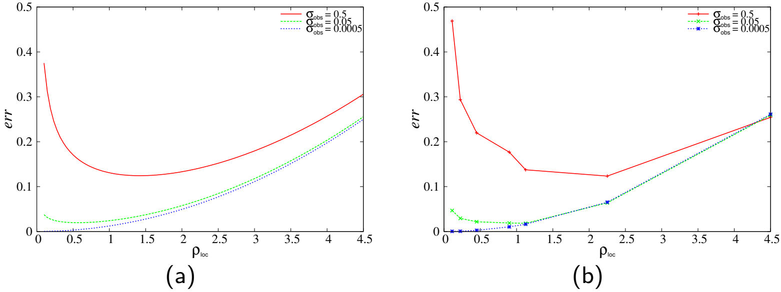
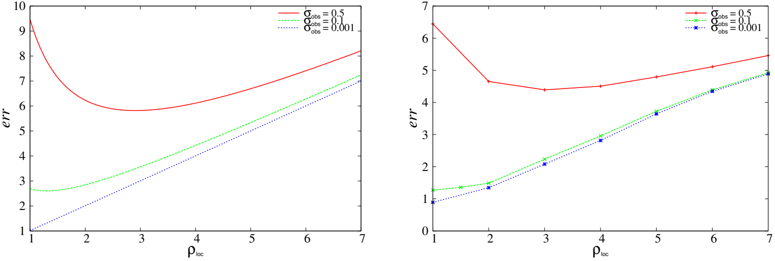


Figure: In (a) we show the theoretical error curve for the case $d = 1$ and $p = 1$. The numerical results (similar curves shown in Greybush et al. 2011) are shown in (b). Here, we display three curves for $\sigma_{obs} \in \{0.0005 \quad 0.05 \quad 0.5\}$.



(a) (b)

Figure: In (a) we show the theoretical error curve for the case $d = 2$ and $p = 1$. Here, we display three curves for $\sigma_{obs} \in \{0.0001 \;\; 0.1 \;\; 0.5\}$.

Outlook / Conclusion

- Optimal localization length ρ_{loc} depending on σ_{obs} and density of observation. These results are analogous for the L95-LETKF.
- For fixed ρ_{loc} in LETKF: $N_{obs} > (N_{ens} - 1)$ gives better results only if ensemble-subspace is appropiated.
- Next steps: Error analysis for **two-step analysis** with different localization radius for each kind of observation assimilated

$$\begin{aligned}
\varphi_1^{(a)} &= \varphi^{(b)} + BH_1^*(R_{1,\rho_1} + H_1 BH_1^*)^{-1}(f_1 - H_1\varphi^{(b)}) \\
\varphi_2^{(a)} &= \varphi_1^{(a)} + B_1 H_2^*(R_{2,\rho_2} + H_2 B_1 H_2^*)^{-1}(f_2 - H_2\varphi_1^{(a)}) \\
\varphi_{total}^{(a)} &= \varphi_2^{(a)}
\end{aligned}$$

- Two-step analysis gives better results if the two observation types have $\sigma_{obs}^1 >> \sigma_{obs}^2$.

Proof of Lemma

Since we have

$$\begin{aligned} \|(f - H\varphi^{(b)}) - HQ_k\gamma\|_{R^{-1}}^2 &= \|(H(\varphi^{(true)} - \varphi^{(b)}) - HQ_k\gamma\|_{R^{-1}}^2 \\ &= \|(\varphi^{(true)} - \varphi^{(b)}) - Q_k\gamma\|_{H^*R^{-1}H}^2 \end{aligned}$$

The element $Q\gamma^{(a)}$ is the *best approximation* in $U^{(L)}$ to the element $\varphi^{(true)} - \varphi^{(b)}$ with respect to the scalar product $\langle \cdot, \cdot \rangle_{H^*R^{-1}H}$.

For the best approximation ψ_* to an element ψ in a Hilbert space X with scalar product $\langle \cdot, \cdot \rangle$ with respect to a finite-dimensional subspace U, for all elements $u \in U$ we have $\langle u, \psi - \psi_* \rangle = 0$.

The analysis $\varphi^{(a)} - \varphi^{(b)} = Q\gamma^{(a)}$ is the orthogonal projection of $\varphi^{(true)} - \varphi^{(b)}$ onto $U_k^{(L)}$.

Finally, we now estimate

$$\begin{aligned} \|\varphi^{(a)} - \varphi^{(true)}\|_{H^* R^{-1} H} &= \|\varphi^{(a)} - \varphi^{(b)} + \varphi^{(b)} - \varphi^{(true)}\|_{H^* R^{-1} H} \\ &= \min_{\gamma} \|Q\gamma - (\varphi^{(true)} - \varphi^{(b)})\|_{H^* R^{-1} H} \\ &= d_{H^* R^{-1} H}\Big(U_k^{(L)}, \varphi^{(true)} - \varphi^{(b)}\Big), \end{aligned}$$

which completes the proof. □

Lemma

Let ψ be a continuously differentiable function defined in some domain V in $\mathbb{R}^n$, $n \in \mathbb{N}$, which satisfies $\psi(x_0) = 0$ for some $x_0 \in V$. Then we have

$$\sup_{x \in B_\rho(x_0)} |\psi(x)| \leq C\rho$$

with the constant $C = \sup_{x \in V} |\nabla \psi(x)|$. In particular, we obtain

$$\sup_{x \in B_\rho(x_0)} |\psi(x)| \ \to 0, \ \ \rho \to 0$$

Proof of Theorem

We carry out the proof for one $x_0 \in V$. We can choose an ensemble member l such that the previous Lemma is satisfied. We set

$$\psi(x) := \frac{|\varphi^{(true)}(x_0) - \varphi^{(b)}(x_0)|}{|\varphi^{(l)}(x_0) - \varphi^{(b)}(x_0|} \left(\varphi^{(l)}(x) - \varphi^{(b)}(x)\right) - \left(\varphi^{(true)}(x) - \varphi^{(b)}(x)\right).$$

yield

$$\sup_{x \in B_\rho(x_0)} |\psi(x)| \leq C\rho \to 0, \quad \rho \to 0.$$

Using the estimate

$$\langle \psi, H^* R^{-1} H\psi \rangle_{B_\rho(x_0)} \leq \|H^*\| \ \|H\| \ \left\|R^{-1}\right\| \langle \psi, \psi \rangle_{B_\rho(x_0)}$$
$$\leq \ \ \|H^*\| \ \|H\| \ \left\|R^{-1}\right\| \ |B_\rho(x_0)| \ \|\psi\|^2_{\infty, B_\rho(x_0)} .$$

Hence, as $\|\psi\|_{\infty, B_\rho(x_0)} = \sup_{x \in B_\rho(x_0)} |\psi(x)| \leq C\rho \to 0, \ \ \rho \to 0.$

This leads to the estimate

$$\|\psi\|^2_{H^* R^{-1} H, \rho} \leq \tau_{H,R} \ \rho \to 0, \ \ \rho \to 0$$

with $\tau_{H,R} := C \|H^*\| \ \|H\| \ \left\|R^{-1}\right\| \ |B_\rho(x_0)|$.

Being ψ the difference between an element in the ensemble space $U^{(L)}$ and $\varphi^{(true)} - \varphi^{(b)}$, we can write

$$\left\| \hat{\varphi}^{(a,\rho)} - \varphi^{(true)} \right\|_{H^* R^{-1} H, \rho} = \left\| \left(\hat{\varphi}^{(a,\rho)} - \varphi^{(b)} \right) - \left(\varphi^{(true)} - \varphi^{(b)} \right) \right\|_{H^* R^{-1} H, \rho}$$

Finally, with the division by $|B_\rho(x_0)|$ now leads to $\hat{E}$ with $\tilde{C} = C \|H^*\| \, \|H\| \, \left\|R^{-1}\right\|$, and the proof is complete. □